

Ballistic-Transport-Induced Negative Differential Thermal Resistance

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Abstract

Using nonequilibrium molecular dynamics simulations, we study the temperature dependence of the negative differential thermal resistance that appears in two-segment Frenkel-Kontorova lattices. We apply the theoretical method based on Landauer equation to obtain the relationship between the heat current and the temperature, which states a fundamental interpret about the underlying physical mechanism of the negative differential thermal resistance. The temperature profiles and transport coefficients are demonstrated to explain the crossover from diffusive to ballistic transport. The finite size effect is also discussed.

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Negative differential thermal resistance (NDTR) is a property of certain materials connected to two heat baths in which, over certain temperature ranges, heat current is a decreasing function of the temperature difference between the two heat baths, i.e., $dJ/dT < 0$, here J and T are the heat current and the temperature, respectively. Li *et al* had investigated different kinds of systems to reveal that negative differential thermal resistance is not a happenstance and indeed take place in low temperature nonlinear lattices for a certain range of parameters [1] [2] [3] [4]. It is naturally expected that NDTR effects may lead to an impressive technological innovation and even the appearance of the thermal transistor, which maybe change our world thoroughly in future, just like electronic transistor and other relevant devices have done in the past half-century [1] [5] [6].

Although thermal transistor is confirmed by nonequilibrium molecular dynamics simulations, the practicable counterpart using fabricated materials is not produced up to now [1]. As the main physical mechanism of thermal transistor, negative differential thermal resistance (NDTR) effect as well as asymmetric heat conductance still need to be understood deeply [7]. The phenomenon of NDTR is firstly understood from the mismatch between the phonon bands of the two interface particles [1]. In Ref. [8] and [9], the authors reported that the phonon bands are independence of the system size but the NDTR disappears for the large system. Segal has suggested that NDTR shows up when the molecular is strongly coupled to the thermal baths in a asymmetric system [4]. However, the NDTR in the absence of asymmetry is still not clear [10]. Therefore, the mismatch of the phonon bands and asymmetry are not a real physical mechanism of the NDTR. To reveal the real physical mechanism of the NDTR is still one of new and challeng-

ing problems about thermal transport.

Macroscopic Fourier's law, $J = -\sigma \nabla T$, that connects heat current with thermal transport on the microscopic scale, is an empirical law based on observation, where ∇T is the temperature gradient and σ is the thermal conductivity. It states that the heat current through a material is proportional to the negative temperature gradient. On the other hand, according to microscopic thermodynamics, heat current at low temperature is proportional to the number of phonons [11]. A phonon is a quantized mode of vibration occurring in a rigid crystal lattice, such as the atomic lattice of a solid [12]. The Bose-Einstein probability distribution for phonons, based on statistical mechanics concepts for thermal equilibrium, determines the number of phonons. Thus, the heat current is also determined by the Bose-Einstein probability distribution. In this paper, applying an analytical method from Landauer equation as well as nonequilibrium molecular dynamics simulations, we reveal the dependence of the NDTR on the temperature and the crossover of two thermal transport processes: the ballistic transport and the diffusive transport [13]. We will also investigate the system size dependence of the NDTR. The temperature profile and the transport coefficient will be calculated to characterize the ballistic transport and the diffusive transport.

The nonlinear lattices that we use in this letter consist of two segments, left segment (L) and right segment (R). Each segment is a Frenkel-Kontorova (F-K) lattice. Segment L and R are coupled via a spring of constant K_{int} . The total Hamiltonian of the model is

$$H = H_L + H_R + H_{int}, \quad (1)$$

and the Hamiltonian of each segment can be written as

$$H_M = \sum_{i=1}^{N_M} \left[\frac{p_{M,i}^2}{2m_M} + \frac{K_M}{2} (q_{M,i+1} - q_{M,i})^2 + \frac{V_M}{(2\pi)^2} \cos\left(\frac{2\pi}{a} q_{M,i}\right) \right], \quad (2)$$

with $q_{M,i}$ and $p_{M,i}$ denote the displacement from equilibrium position and the conjugate momentum of the i^{th} particle in segment M , where M stands for L or R . The parameters K and V are the harmonic spring constant and the strength of the external potential of the FK lattice, respectively. We couple the last particle of segment L and R via a harmonic spring. Thus, $H_{int} = \frac{K_{int}}{2} (q_{L,N} - q_{R,N})^2$. We set $m = a = 1$, $K_L = 1.0$, $K_R = 0.2$, $V_L = 5.0$, $V_R = 1.0$, $K_{int} = 0.05$.

In our simulations we use fixed boundary condition and the chain is connected to two heat baths at temperature T_L and T_R . We use the Nosé-Hoover heat baths and integrate the equations of motion by using the fourth-order Runge-Kutta algorithm [14] [15] [16]. The local temperature is defined as $T_i = \langle p_i^2 \rangle$. The local heat flux is defined as $j_i = K_M \langle p_i (q_i - q_{i-1}) \rangle$, and the total heat flux is $J = Nj$. The simulations are performed long enough to allow the system to reach a steady state in which the local heat flux is constant along the chain. For the sake of comparison, we define a heat current ratio, $J_R = J/J_{\max}$, in which J_{\max} is the maximum heat current under a fixed temperature T_R of the right heat bath. The transport coefficient is an important quantity for characterizing the transport mode of a thermal transport process [17] [18] [19]. The thermal conductance evaluated as $\sigma = Nj/\Delta T$ represents an effective transport coefficient that includes both boundary and bulk resistances [20].

Figure 1 displays a typical negative differential thermal resistance [1]. When the temperature difference increases (i.e., $T_L (\leq T_R)$ decreases), the heat current increases firstly and then decreases. The former is positive differential thermal resistance (PDTR) and the latter negative differential thermal resistance. It would be much interesting to show the thermal conductance dependent behavior of NDTR, which is also presented in Fig.1. It is clearly that the NDTR corresponds to the ballistic regime and PDTR the diffusive regime.

The phenomenon of NDTR can be understood from the theoretical approach. We use Landauer equation to calculate the heat flux. For example, in the ballistic regime the phonon heat flux can be also calculated through a Landauer type expression [21]:

$$J = \int d\omega \omega \chi(\omega) [n_R(\omega) - n_L(\omega)], \quad (3)$$

where $\chi(\omega)$ is the temperature independent transmission coefficient for phonons of frequency ω . Here $n_M(\omega) = (e^{\beta_M \omega} - 1)^{-1}$, $\beta_M = 1/k_B T_M$, ($M = L, R$) is the Bose-Einstein distribution characterizing the heat baths.

As reported in Ref.[4], under the assumption of weak system-bath interactions and when going into the Marko-

FIG. 1: The temperature dependence of heat current ratio (blank squares) and the corresponding temperature dependence of the thermal conductance (solid circles). The system parameters are $N_L = N_R = 50$, $V_L = 5.0$, $V_R = 1.0$, $K_L = 1.0$, $K_R = 0.2$, $K_{int} = 0.05$, and $T_R = 0.21$.

vian limit, the probabilities P_n to occupy the n state of the phonon are found to satisfy the master equation

$$\dot{P}_n = (n+1)k_d P_{n+1} + nk_u P_{n-1} - [nk_d + (n+1)k_u] P_n, \quad (4)$$

here the occupations are normalized $\sum P_n = 1$, and k_d and k_u are the vibrational relaxation and excitation rates, respectively.

When going into weak system-bath interaction, k_d and k_u can satisfy:

$$k_d = k_L + k_R, k_u = k_L e^{-\beta_L \omega_0} + k_R e^{-\beta_R \omega_0}, \quad (5)$$

with $k_M = \Gamma_M(\omega)[1 + n_M(\omega_0)]$, where $n_M(\omega) = (e^{\beta_M \omega} - 1)^{-1}$, $\Gamma_M(\omega) = \frac{\pi}{2m\omega^2} \sum \alpha_j^2 \delta(\omega - \omega_j)$ and $\alpha_j = \bar{\alpha}_j \sqrt{2m\omega_0}$, here, m , ω_0 , $\bar{\alpha}_j$ are molecular oscillator mass, frequency and coupling between the system and the heat baths, respectively.

The thermal properties of our model are obtained from the stationary state solution of Eq.(4). The thermal flux is given by

$$J = \omega_0 \sum n(k_L P_n - k_L P_{n-1} e^{-\beta_L \omega_0}). \quad (6)$$

here positive sign denotes current flowing from right to left. In this equation the first term indicates the thermal flux flowing from the L chains into the L heat bath. The

second term gives the oppositely flowing flux from L heat bath to the chain. The thermal flux could be equivalently calculated at the R chain.

So for the asymmetry system, which is similar to the case of a highly anharmonic molecule coupled-possible asymmetrically-but linearly, to two heat baths of different temperatures. Here, we simulate strong anharmonicity by modeling the anharmonic two-segment chains by a two levels system that notes a highly anharmonic vibrational mode [4]. The Hamiltonian for this model is the same as presented in Eq.(1), except that we take $n = 0, 1$ only. Following Eq.(3)- (6) and going into the classical limit, the heat current reduces into the simple form

$$J = \omega_0 \frac{\Gamma_L \Gamma_R (n_R - n_L)}{\Gamma_L (1 + 2n_L) + \Gamma_R (1 + 2n_R)} \quad (7)$$

$$= \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \frac{\omega_0}{T_s} (T_R - T_L) [\exp(\omega_0/T_s) + 1]^{-1}, \quad (8)$$

in which

$$T_s = \frac{\Gamma_L T_L + \Gamma_R T_R}{\Gamma_L + \Gamma_R}. \quad (9)$$

We can now clearly seek the main factors which influence the heat current. The thermal flux is given by multiplying four terms: (1) A symmetric prefactor $\Gamma_L \Gamma_R / (\Gamma_L + \Gamma_R)$. (2) The characteristic frequency and effective temperature ω_0/T_s . (3) The temperature difference $(T_R - T_L)$. (4) The molecular occupation factor $[\exp(\omega_0/T_s) + 1]^{-1}$ [4]. This expression denotes that the heat current is mainly a competitive effect between the temperature difference and the molecular occupation factor. In the case of low temperature (i.e., in the ballistic regime), the molecular occupation factor changes obviously with T_s by going into an exponential function, while in the case of high temperature ($T_s \gg \omega_0$, indicates the diffusive regime) the molecular occupation factor is a constant $1/2$.

Figure 2 shows the simulated results of the temperature dependence of NDTR. When T_R is small, there exists NDTR. As T_R increases, however, the NDTR disappears. As also shown in Fig.3, a theoretical estimation Eq.(8) based on Landauer equation confirms this temperature dependence of NDTR simultaneously.

Why does the NDTR appear at low temperature and disappear at high temperature? This phenomenon can be also understood in detail from the crossover from the diffusive to ballistic transport. In the case of low temperature T_R , as shown in Fig.4a, when T_L changes from T_R to zero, the temperature profiles of the lattices illustrate a zero temperature gradient. This diffusive-ballistic transition with temperature difference is also shown in Fig.4b. When the temperature difference is small, the thermal conductance does not change with T_L . However, when the temperature difference is large, the thermal conductance decreases linearly with T_L decreasing.

FIG. 2: Heat current ratio as a function of the temperature T_L for $T_R=0.11, 0.31, 0.51$, and 1.01 . The system parameters are $V_L = 5.0$, $V_R = 1.0$, $K_L = 1.0$, $K_R = 0.2$, $K_{int} = 0.05$, and $N_L=N_R=50$.

FIG. 3: The temperature dependence of heat current. Results are obtained from Eq.(8) with $T_R=200\text{K}$ (full), 100K (dash), 50K (dot). The remain parameters are $\omega_0 = 150\text{meV}$, $\Gamma_L = 1.0\text{meV}$, $\Gamma_R = 1.4\text{meV}$.

FIG. 4: (a) Temperature profiles of the lattices for different heat baths for $T_L=0.02$. (b) Thermal conductance as a function of the temperature T_L/T_R for different temperatures $T_R=0.11, 0.21, 0.41, 0.81$ and 1.01 (from bottom to top). Remain parameters are the same as for Fig.2.

It can be interpreted that the diffusive-ballistic transition induces the NDTR, which takes place just when the ballistic transport prevails over the diffusive transport. In the case of high temperature T_R , even when T_L is very small, the temperature gradient are non-zero and the thermal conductance does not change with T_L . There exists no diffusive-ballistic transition. Therefore, the NDTR does not occur in the case of high temperature T_R .

We would also like to discuss the finite size effect of NDTR. As shown in Ref. [9]. When the system size increases, the phenomenon of NDTR disappears. It is interesting to present the system size dependence of thermal conductance, which is shown in Fig.5. In the ballistic regime (i.e., when the system size is much smaller than the phonon mean free path), thermal conductance increases linearly with the system size. In the diffusive regime (i.e., when the system size increases to far larger than the phonon mean free path), thermal conductance will be independence of the system size. There exists a crossover from ballistic to diffusive transport with the increase of the system size. When the system goes to completely diffusive transport regime, the temperature difference does not change the transport mode and then the NDTR disappears.

FIG. 5: Thermal conductance versus lattice length $N(= N_L + N_R)$ for $T_R = 0.21$ and $T_L = 0.05$ (Triangles), 0.07 (Circles), and 0.15 (Squares). Remain parameters are the same as for Fig.2.

In conclusions, we have found the physical mechanism of the negative differential thermal resistance in two-segment asymmetric F-K chains through both theoretical analyses and numerical simulations. From the analytical relationship between the heat current and the temperature, the NDTR effect can be understood from a competition between the temperature difference and the molecular occupation factor. In the ballistic regime the molecular occupation factor mainly depends seriously on the temperature. However, in the diffusive regime, the molecular occupation factor is a constant. The NDTR effect occurs just because the decrease of the molecular occupation factor is faster than the increase of the temperature difference. The main factors that influence the transport modes of the phonons are the temperature and the system size. We propose that different system structures can affect the temperature dependence of NDTR through changing the transmission mode of the phonons. When there exists a crossover from diffusive to ballistic transport, the NDTR can be observed, otherwise it will not. Due to the rigorous condition of validity: low temperature and small system, we still have a long way to go before the NDTR effect is produced in fabricated materials.

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